



Module **PMRF-ISSS150/III/2024**

Basics of Computational Chemistry

Name of the PMRF student

Ritwika Chatterjee

Required background of the students taught

Basics of Quantum Mechanics is desired

3rd/4th year UG or PG students

Details of the content of the module

- **Concepts of Computational Modelling**

Potential Energy Surface, Born-Oppenheimer Approximation, Stationary Points, Geometry Optimization, Normal-Mode Vibrations

- **Molecular Mechanics**

Basic Principles, Force Fields, Basics of Molecular Dynamics Simulations

- **Ab Initio Methods**

Hartree-Fock Method, Basis Sets

- **Density Functional Theory**

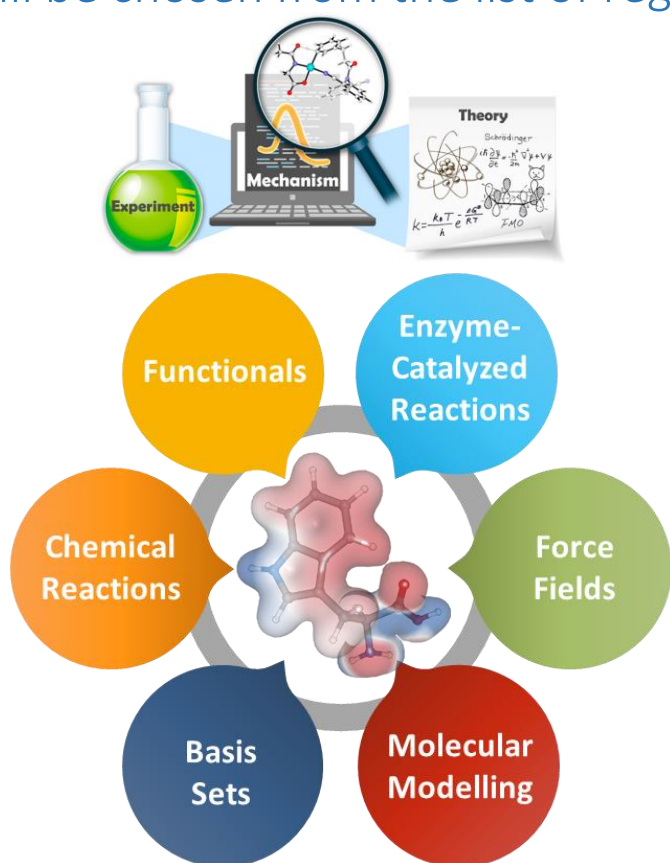
Foundation, Kohn-Sham Self-consistent Field Method, Exchange-correlation Functionals

- **Hybrid Quantum/Classical Methods**

Applications in Enzymatic Systems

Online session coordinator

Will be chosen from the list of registrants



Schedule of the module

Start Date: **01/10/2024**

End Date: 31/12/2024 tentatively)

Class Timing: Monday and Wednesday, 6 PM (1hour)

Meeting link : Will be shared later

Contact email ID: iss.forum@gmail.com

Registration link: Click [HERE](#)